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PASSWORD:
TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page URLs for STN Seminar Schedule - N. America
NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005
NEWS	19	FEB 16	STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005
NEWS	20	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	21	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	22	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	23	MAR 02	GBFULL: New full-text patent database on STN
NEWS	24	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	25	MAR 03	MEDLINE file segment of TOXCENTER reloaded

NEWS EXPRESS	JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN

NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:16:29 ON 14 MAR 2005

=>
Uploading
THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE
Do you want to switch to the Registry File?
Choice (Y/n):
Switching to the Registry File...
Some commands only work in certain files. For example, the EXPAND command can only be used to look at the index in a file which has an index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:16:38 ON 14 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1
DICTIONARY FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

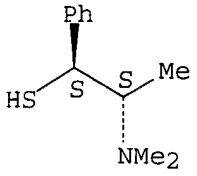
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10807710.str

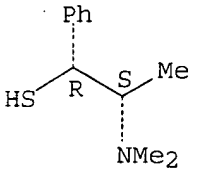
α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, L(+)-threo-
(preparation of)
RN 942-48-3 CAPLUS
CN Benzenemethanethiol, α-[1-(dimethylamino)ethyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



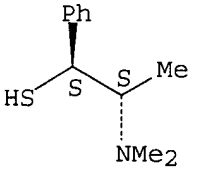
RN 942-49-4 CAPLUS
CN α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, L-(-)-erythro- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



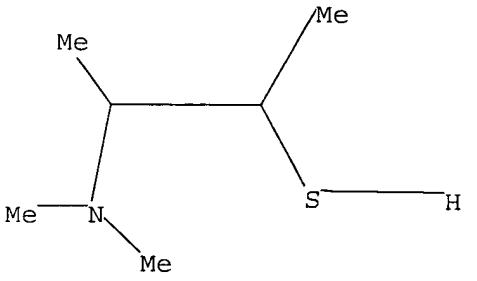
RN 942-50-7 CAPLUS
CN Benzenemethanethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

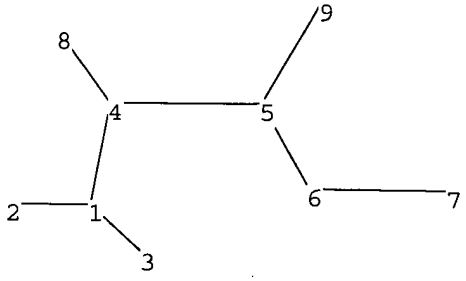
Absolute stereochemistry.



● HCl

L13 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:447807 CAPLUS
DOCUMENT NUMBER: 61:47807
ORIGINAL REFERENCE NO.: 61:8284a-b
TITLE: Preparation of quaternary ammonium betaine salts
INVENTOR(S): Klass, Donald L.
PATENT ASSIGNEE(S): Pure Oil Co.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent



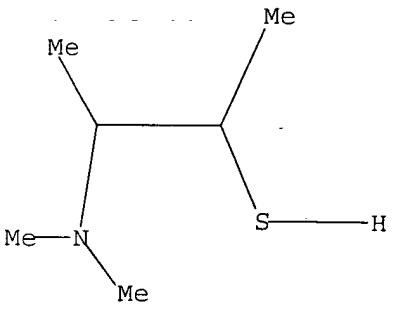


chain nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-2 1-3 1-4 4-5 4-8 5-6 5-9 6-7
exact/norm bonds :
1-4 5-6
exact bonds :
1-2 1-3 4-5 4-8 5-9 6-7

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L1 STRUCTURE UPLOADED

=> D L1
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1
SAMPLE SEARCH INITIATED 14:16:51 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1948 TO ITERATE

51.3% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**
PROJECTED ITERATIONS: 36313 TO 41607
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> S L1 SSS FULL
FULL SEARCH INITIATED 14:16:58 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 37690 TO ITERATE

100.0% PROCESSED 37690 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

L3 4 SEA SSS FUL L1

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	161.54

FILE 'CAPLUS' ENTERED AT 14:17:04 ON 14 MAR 2005
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FILE COVERS 1907 - 14 Mar 2005 VOL 142 ISS 12
FILE LAST UPDATED: 13 Mar 2005 (20050313/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> S L3
L4 3 L3

=> d l4 ibib abs hitstr tot

L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2005:141013 CAPLUS
DOCUMENT NUMBER: 142:212335
TITLE: Polyamine and aminothiol compounds and compositions for use in conjunction with cancer therapy
INVENTOR(S): Fahl, William E.; Peebles, Daniel D.; Copp, Richard R.
PATENT ASSIGNEE(S): Wisconsin Alumni Research Foundation, USA
SOURCE: PCT Int. Appl., 142 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005014524	A2	20050217	WO 2004-US26535	20040809

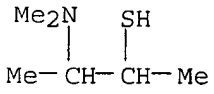
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-493218P P 20030807

AB The invention provides polyamine and aminothiol compds. and pharmaceutical compns. for administration in conjunction with cancer chemotherapy or radiation therapy. The compds. are administered locally to provide protection against the adverse side-effects of chemotherapy or radiation therapy, such as alopecia, mucositis and dermatitis. Pharmaceutical prepns. comprising one or more chemoprotective polyamines or aminothiols formulated for topical or local delivery to epithelial or mucosal cells are disclosed. Methods of administering the pharmaceutical prepns. are also disclosed.

IT **844435-75-2**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(polyamine and aminothiol compds. and compns. for use in conjunction with cancer therapy)

RN 844435-75-2 CAPLUS
CN 2-Butanethiol, 3-(dimethylamino)- (9CI) (CA INDEX NAME)



L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:562548 CAPLUS
DOCUMENT NUMBER: 101:162548
TITLE: Substituted cysteamine ligands and their complexes with molybdenum(VI)
AUTHOR(S): Corbin, James L.; Miller, Kenneth F.; Pariyadath, Narayanakutty; Heinecke, Jay; Bruce, Alice E.; Wherland, Scot; Stiefel, Edward I.
CORPORATE SOURCE: Charles F. Kettering Res. Lab., Yellow Springs, OH, 45387, USA
SOURCE: Inorganic Chemistry (1984), 23(21), 3404-12
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

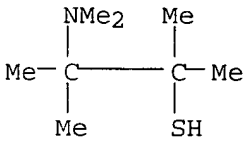
AB New bidentate cysteamine-based ligands containing Me-substituted C and N atoms were prepared Together with known ligands the following complete set has now been prepared: NH2CH2CH2SH, MeNHCH2CH2SH, Me2NCH2CH2SH, NH2C(CH3)2CH2SH,

MeNHC(CH3)2CH2SH, Me2NC(CH3)2CH2SH, NH2CH2C(CH3)2SH, MeNHCH2C(CH3)2SH, Me2NCH2C(CH3)2SH, NH2C(CH3)2C(CH3)2SH, MeNHC(CH3)2C(CH3)2SH, and Me2NC(CH3)2C(CH3)2SH. Five of the ligands in this series are new, and their preparation is reported in detail. Also RNHCH2C(CH3)2SH ligands (R = iso-Pr and iso-Bu) are reported for the 1st time. These ligands, LH, were reacted in MeOH with MoO2(acac)2 (Hacac = acetylacetone). In most cases MoO2L2 resulted. However, in some cases this complex appears to be unstable. The prepns. and spectroscopic properties of the complexes are reported. The low values of ν(Mo-O) for some of the complexes are correlated either with H bonding or with the presence of a skew-trapezoidal-bipyramidal structure. Likewise, electronic absorption spectra differ for complexes with octahedral as opposed to skew-trapezoidal-bipyramidal structures. For a given complex, 17O and 1H NMR spectroscopies are consistent with adoption in solution of the same octahedral or skew-trapezoidal-bipyramidal structure that is found in the solid state. Further, the skew-trapezoidal-bipyramidal complexes display temperature-dependent NMR spectra that are interpreted in terms of configurational averaging probably caused by Mo-N bond cleavage.

IT **91229-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 91229-44-6 CAPLUS

CN 2-Butanethiol, 3-(dimethylamino)-2,3-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1964:447807 CAPLUS
DOCUMENT NUMBER: 61:47807
ORIGINAL REFERENCE NO.: 61:8284a-b
TITLE: Preparation of quaternary ammonium betaine salts
INVENTOR(S): Klass, Donald L.
PATENT ASSIGNEE(S): Pure Oil Co.
SOURCE: 4 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3131189		19640428	US	19611016

GI For diagram(s), see printed CA Issue.

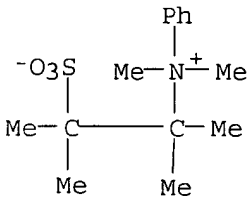
AB Carbyl sulfate (I), prepared by the reaction of 2 moles SO3 and 1 mole ethylene, reacted with a tertiary amine to form betaines. Thus 1.5 g. pyridine (II) in 10 ml. ethylene dichloride was added to 3 g. I in 30 ml. ethylene dichloride (the reaction was exothermic), the liquid decanted from the precipitate, and the precipitate covered with petr. ether and cooled to give

IIa (R = R1 = H), m. 250-5° (HCONMe2). I was also treated with the following to form betaines: quinoline, acridine, trimethylamine, and dimethylaniline (III). Also reported without details were: IIa (R = Ph, R1 = H); Et3NCHEtCH2SO3; IIa (R = R1 = Me); and PhNMe2CMe2CMe2SO3. These compds. are useful intermediates for the preparation of detergents. (Cf. U.S. 2,666,788, or Brit. 686,061.)

IT **97176-62-0**, Ammonium, dimethylphenyl(1,1,2-trimethyl-2-sulfopropyl), hydroxide, inner salt
(preparation of)

RN 97176-62-0 CAPLUS

CN Dimethylphenyl(1,1,2-trimethyl-2-sulfopropyl)ammonium hydroxide, inner salt (7CI) (CA INDEX NAME)



=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	18.42	179.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-2.19	-2.19

FILE 'REGISTRY' ENTERED AT 14:21:56 ON 14 MAR 2005
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STRUCTURE FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1
DICTIONARY FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1

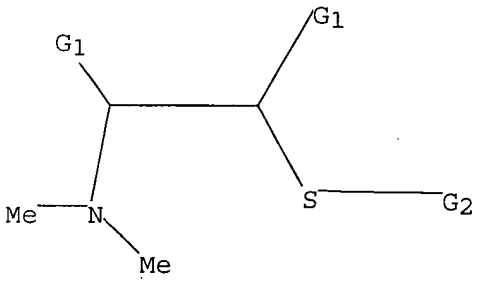
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

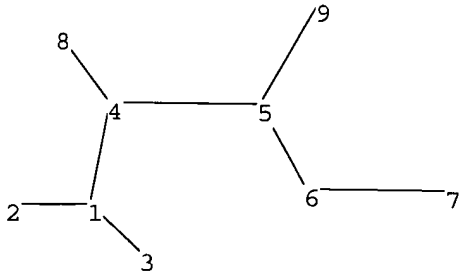
Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10807710a.str





chain nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-2 1-3 1-4 4-5 4-8 5-6 5-9 6-7
exact/norm bonds :
1-4 4-8 5-6 5-9 6-7
exact bonds :
1-2 1-3 4-5

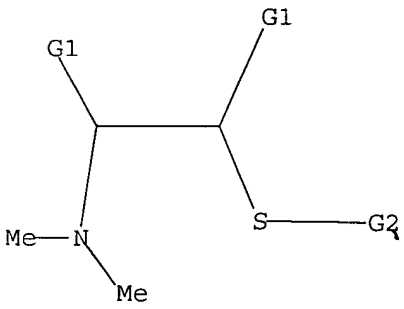
G1:Ak,Ph

G2:H,CH3

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS

L5 STRUCTURE UPLOADED

=> d l5
L5 HAS NO ANSWERS
L5 STR



G1 Ak,Ph
G2 H,Me

Structure attributes must be viewed using STN Express query preparation.

=> s l5
SAMPLE SEARCH INITIATED 14:22:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 5592 TO ITERATE

17.9% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 107357 TO 116323
PROJECTED ANSWERS: 0 TO 0

L6 0 SEA SSS SAM L5

=> s l5 sss full
FULL SEARCH INITIATED 14:22:26 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 109275 TO ITERATE

100.0% PROCESSED 109275 ITERATIONS 36 ANSWERS
SEARCH TIME: 00.00.02

L7 36 SEA SSS FUL L5

=> FIL CAPLUS

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	341.29

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.19

FILE 'CAPLUS' ENTERED AT 14:22:37 ON 14 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 14 Mar 2005 VOL 142 ISS 12
FILE LAST UPDATED: 13 Mar 2005 (20050313/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l7
L8 18 L7

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION

FULL ESTIMATED COST 1.80 343.09

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE ENTRY TOTAL SESSION

CA SUBSCRIBER PRICE 0.00 -2.19

FILE 'REGISTRY' ENTERED AT 14:24:46 ON 14 MAR 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1
DICTIONARY FILE UPDATES: 13 MAR 2005 HIGHEST RN 845467-46-1

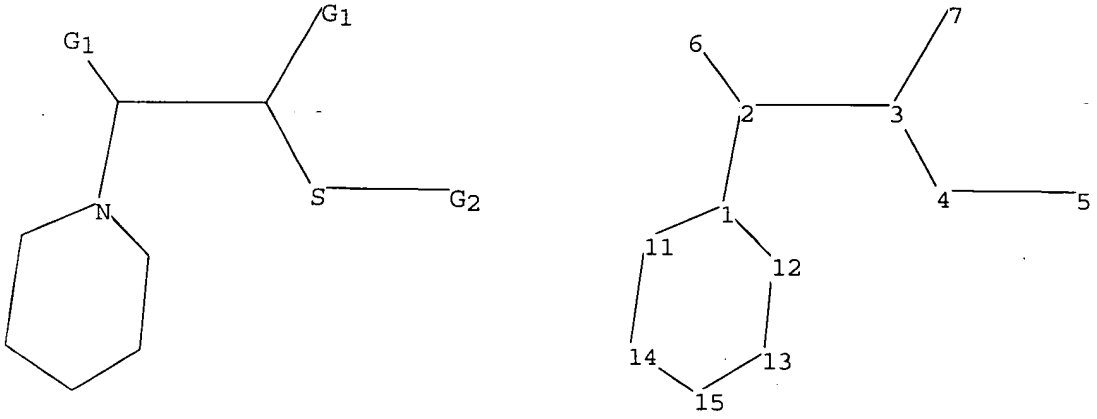
TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10807710b.str



chain nodes :
2 3 4 5 6 7
ring nodes :
1 11 12 13 14 15
chain bonds :
1-2 2-3 2-6 3-4 3-7 4-5
ring bonds :
1-11 1-12 11-14 12-13 13-15 14-15
exact/norm bonds :
1-2 1-11 1-12 2-6 3-4 3-7 4-5 11-14 12-13 13-15 14-15
exact bonds :
2-3

isolated ring systems :
containing 1 :

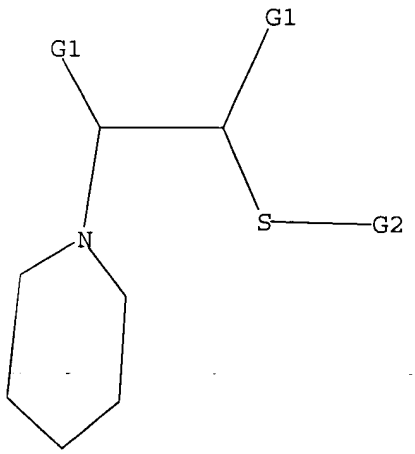
G1:Ak,Ph

G2:H,CH3

Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 11:CLASS 12:CLASS
13:CLASS 14:CLASS 15:CLASS

L9 STRUCTURE UPLOADED

=> d l9
L9 HAS NO ANSWERS
L9 STR



G1 Ak,Ph
G2 H,Me

Structure attributes must be viewed using STN Express query preparation.

=> s l9
SAMPLE SEARCH INITIATED 14:25:15 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3163 TO ITERATE

31.6% PROCESSED 1000 ITERATIONS 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 59887 TO 66633
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=> s l9 sss full
FULL SEARCH INITIATED 14:25:23 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 62510 TO ITERATE

100.0% PROCESSED 62510 ITERATIONS 17 ANSWERS
SEARCH TIME: 00.00.01

L11 17 SEA SSS FUL L9

=> FIL CAPLUS
COST IN U.S. DOLLARS

	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	161.33	504.42

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-2.19

FILE 'CAPLUS' ENTERED AT 14:25:32 ON 14 MAR 2005
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FILE COVERS 1907 - 14 Mar 2005 VOL 142 ISS 12
FILE LAST UPDATED: 13 Mar 2005 (20050313/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 14:16:29 ON 14 MAR 2005)

FILE 'REGISTRY' ENTERED AT 14:16:38 ON 14 MAR 2005
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 4 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 14:17:04 ON 14 MAR 2005
L4 3 S L3

FILE 'REGISTRY' ENTERED AT 14:21:56 ON 14 MAR 2005
L5 STRUCTURE UPLOADED
L6 0 S L5
L7 36 S L5 SSS FULL

FILE 'CAPLUS' ENTERED AT 14:22:37 ON 14 MAR 2005
L8 18 S L7

FILE 'REGISTRY' ENTERED AT 14:24:46 ON 14 MAR 2005
L9 STRUCTURE UPLOADED
L10 0 S L9
L11 17 S L9 SSS FULL

FILE 'CAPLUS' ENTERED AT 14:25:32 ON 14 MAR 2005

=> s l11
L12 20 L11

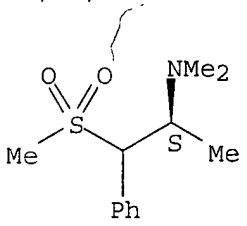
=> s l8 and py<=2002
22589460 PY<=2002
L13 17 L8 AND PY<=2002

=> s l12 and py<=2002
22589460 PY<=2002
L14 17 L12 AND PY<=2002

=> d l13 ibib abs hitstr tot

L13 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:671830 CAPLUS
DOCUMENT NUMBER: 132:35935
TITLE: Diastereomeric sulfinates derived from (L)-N-methylephedrine: synthesis, applications and rearrangements
AUTHOR(S): Drabowicz, Jozef; Bujnicki, Bogdan; Biscarini, Paolo; Mikolajczyk, Marian
CORPORATE SOURCE: Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Lodz, 90-363, Pol.
SOURCE: Tetrahedron: Asymmetry (**1999**), 10(16), 3177-3187
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:35935
AB The reaction of sulfinyl chlorides with (L)-N-methylephedrine alone or in the presence of tertiary amines was found to produce diastereomeric sulfinates with diastereomeric purities up to 90%. The diastereomeric ratio is strongly influenced by the nature of substituents on the sulfinyl chlorides and to some extent by the reaction conditions. In a few cases, the pure diastereomers were isolated by chromatog. and used for the preparation of optically active sulfoxides. The silica gel catalyzed rearrangement of sulfinates to the corresponding sulfones is also discussed.
IT **252230-36-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(diastereomeric sulfinates derived from (L)-N-methylephedrine, synthesis, applications and rearrangements)
RN 252230-36-7 CAPLUS
CN Benzeneethanamine, N,N,α-trimethyl-β-(methylsulfonyl)-, (αS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



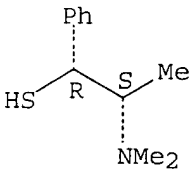
REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L13 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:809918 CAPLUS
DOCUMENT NUMBER: 123:286349
TITLE: Thiol and disulfide derivatives of Ephedra alkaloids. 2. A mechanistic study of their effect on the addition of diethylzinc to benzaldehyde
AUTHOR(S): Fitzpatrick, Kevin; Hulst, Ron; Kellogg, Richard M.
CORPORATE SOURCE: Dep. of Organic and Molecular Inorganic Chem., Univ. of Groningen, Groningen, 9747 AG, Neth.
SOURCE: Tetrahedron: Asymmetry (**1995**), 6(8), 1861-4
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:286349

AB Non-linear correlations between the ee of the product, PhCH(OH)Et, and the catalyst, ephedrine thiol or disulfide derivs., were observed Osmotic measurements indicate a high degree of aggregation of the Zn thiolates. The behavior of the thiol derivs. deviates sharply from that of N-methylephedrine.

IT **2218-21-5**
RL: CAT (Catalyst use); USES (Uses)
(effect of thiol and disulfide derivs. of ephedrine on addition of Et2Zn to benzaldehyde)
RN 2218-21-5 CAPLUS
CN Benzenemethanethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

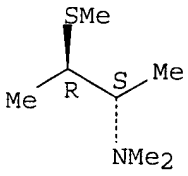
L13 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:531411 CAPLUS
DOCUMENT NUMBER: 113:131411
TITLE: Concerning mass spectra of β-heterosubstituted thioethers

AUTHOR(S): Carreno, M. Carmen; Carretero, Juan C.; Garcia Ruano, Jose L.; Martinez, M. Carmen
CORPORATE SOURCE: Dep. Quim., Univ. Auton. Madrid, Madrid, 28049, Spain
SOURCE: Organic Mass Spectrometry (**1990**), 25(6), 339-42
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mass spectra of 32 erythro- and threo-RCHXCHRSMe (R = Me, Ph; X = F, Cl, Br, iodo, OH, OMe, OAc, NH2, NMe2) were interpreted in detail. Linear free-energy relationships were determined between the ratio of the relative abundances of the RCHX+ and RCHSMe+ peaks and the inductive and resonance σ consts. of X.

IT **97241-41-3 97241-45-7 97241-46-8**
97241-47-9
RL: PRP (Properties)
(mass spectrum of)

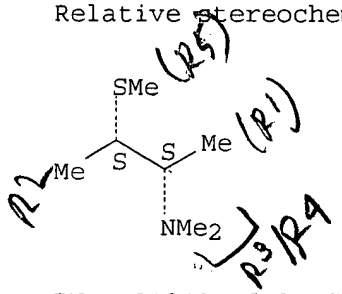
RN 97241-41-3 CAPLUS
CN 2-Butanamine, N,N-dimethyl-3-(methylthio)-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



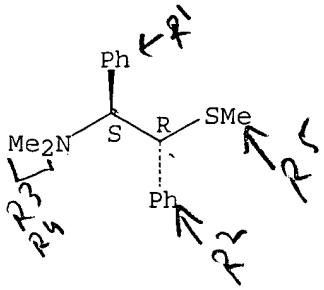
RN 97241-45-7 CAPLUS
CN 2-Butanamine, N,N-dimethyl-3-(methylthio)-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



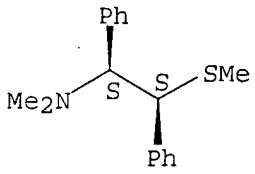
RN 97241-46-8 CAPLUS
CN Benzeneethanamine, N,N-dimethyl-β-(methylthio)-α-phenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 97241-47-9 CAPLUS
CN Benzeneethanamine, N,N-dimethyl-β-(methylthio)-α-phenyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

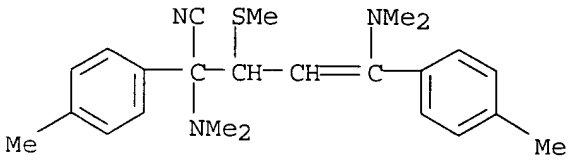


L13 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:458617 CAPLUS
DOCUMENT NUMBER: 113:58617
TITLE: Reactions of organic anions. 168. Reactions of 2-(dialkylamino)arylacetonitriles with acetylenes under basic conditions. A simple synthesis of substituted mono- and diketones
AUTHOR(S): Zdrojewski, T.; Jonczyk, A.
CORPORATE SOURCE: Dep. Chem., Tech. Univ., Warsaw, PL-00-662, Pol.
SOURCE: Synthesis (**1990**), (3), 224-33
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:58617

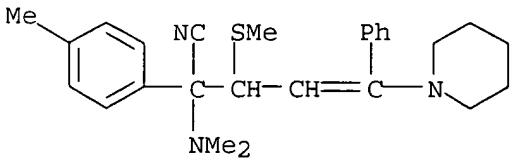
AB The reaction of RCH(CN)NR12 (I; R = Ph, 4-MeC6H4, 4-MeOC6H4; R1 = Me; NR12 = piperidino, morpholino, etc.) with R2C.tplbond.CH (II; R2 = Ph, MeS) gave R12NCR(CN)CH:CHR2 (III) and/or R12NCR(CN)CHR2CH:CRNR12; the product depended on the basicity of the amino group in III. I also added to C-1 of II (R2 = EtO) to give R12NCR(CN)C(OEt):CH2. All these products could be hydrolyzed to give mono- or diketones.

IT **128407-41-0P 128407-44-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

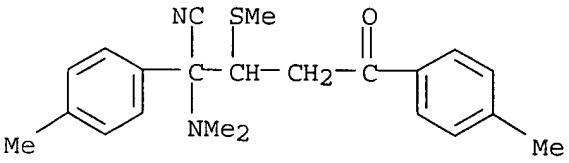
RN 128407-41-0 CAPLUS
CN Benzeneacetonitrile, α-(dimethylamino)-α-[3-(dimethylamino)-3-(4-methylphenyl)-1-(methylthio)-2-propenyl]-4-methyl- (9CI) (CA INDEX NAME)



RN 128407-44-3 CAPLUS
CN Benzeneacetonitrile, α-(dimethylamino)-4-methyl-α-[1-(methylthio)-3-phenyl-3-(1-piperidinyl)-2-propenyl]- (9CI) (CA INDEX NAME)



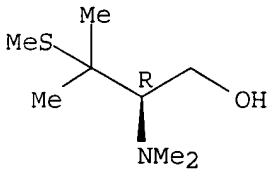
IT **128407-50-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 128407-50-1 CAPLUS
CN Benzenepentanenitrile, α-(dimethylamino)-4-methyl-α-(4-methylphenyl)-β-(methylthio)-δ-oxo- (9CI) (CA INDEX NAME)



L13 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:505278 CAPLUS
DOCUMENT NUMBER: 103:105278
TITLE: L-Cysteine-, L-methionine- and D-penicillamine-derived ligands for transition metal catalyzed carbon-carbon bond-forming reactions
AUTHOR(S): Griffin, John H.; Kellogg, Richard M.
CORPORATE SOURCE: Dep. Org. Chem., Univ. Groningen, Groningen, 9747 AG, Neth.
SOURCE: Journal of Organic Chemistry (**1985**), 50(18), 3261-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:105278
AB L-Cysteine, L-methionine, and D-penicillamine were converted to their corresponding S-alkylated dimethylamino alcs. by alkylation of sulfur and nitrogen followed by reduction of the carboxyl group. One-pot mesylation followed by treatment with lithium diphenylphosphide provides the corresponding phosphine derivative, 2-(dimethylamino)-1-(diphenylphosphino)-3-(methylthio)propane (cysphos), the S-iso-Pr derivative (isopropylcycphos), 2-(dimethylamino)-1-(diphenylphosphino)-4-(methylthio)butane (methphos), and 2-(dimethylamino)-1-(diphenylphosphino)-3-methyl-3-(methylthio)butane (penphos). The latter ligand had an enantiomeric excess of 82%, whereas the other ligands are enantiomerically pure. These compds. were used as ligands for the solubilization of catalytic amts. of NiCl2, which is used to mediate the coupling of vinyl bromide with the (racemic) Grignard reagent or 1-phenyl-1-chloroethane to give 3-phenyl-1-butene in excellent yields and with enantiomeric excesses of up to 65% (methphos). The cross coupling of vinyl bromide to the Grignard reagent of 2-octyl chloride was also examined; enantiomeric excesses of 3-methyl-1-nonene of up to 18% are obtained (penphos).
IT **97071-94-8P 97072-02-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)

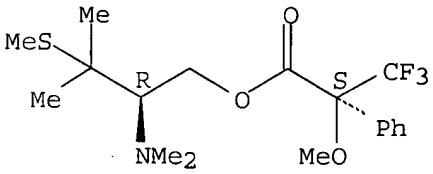
(preparation of)
RN 97071-94-8 CAPLUS
CN 1-Butanol, 2-(dimethylamino)-3-methyl-3-(methylthio)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



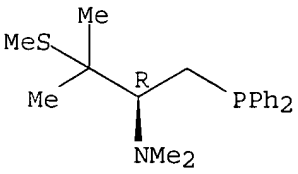
RN 97072-02-1 CAPLUS
CN Benzeneacetic acid, α-methoxy-α-(trifluoromethyl)-, 2-(dimethylamino)-3-methyl-3-(methylthio)butyl ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **97071-99-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as ligand for asym. nickel-catalyzed crosscoupling of Grignard reagents with vinyl bromide)
RN 97071-99-3 CAPLUS
CN 2-Butanamine, 1-(diphenylphosphino)-N,N,3-trimethyl-3-(methylthio)-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:437072 CAPLUS
DOCUMENT NUMBER: 103:37072
TITLE: Syntheses of β-heterosubstituted thioethers
AUTHOR(S): Carretero, J. Carlos; Garcia-Ruano, Jose L.; Martinez, M. Carmen; Rodriguez, Jesus H.
CORPORATE SOURCE: Dep. Quim. Org., Univ. Auton. Madrid, Madrid, 28049, Spain
SOURCE: Journal of Chemical Research, Synopses (**1985**), (1), 6-7

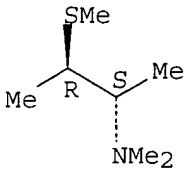
CODEN: JRPSDC; ISSN: 0308-2342
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 103:37072

AB The thio ethers erythro- and threo-RCHR1CHRSMe (I; R = Me, Ph; R1 = OH, OMe, F, Cl, Br, iodo, NH2, NMe2) were prepared starting from readily available substrates. I (R = Me, R1 = OH) were readily prepared by treatment of the corresponding MeCHBrCHMeOH with NaSMe in MeOH at 0° for 3 h; the reaction occurs with retention of configuration. Treatment of I (R = Me, R1 = OH) with HCl(g) in CHCl3 at room temperature gave the corresponding I (R = Me, R1 = Cl).

IT **97241-41-3P 97241-45-7P 97241-46-8P 97241-47-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

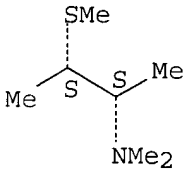
RN 97241-41-3 CAPLUS
CN 2-Butanamine, N,N-dimethyl-3-(methylthio)-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



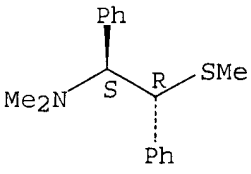
RN 97241-45-7 CAPLUS
CN 2-Butanamine, N,N-dimethyl-3-(methylthio)-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 97241-46-8 CAPLUS
CN Benzeneethanamine, N,N-dimethyl-β-(methylthio)-α-phenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

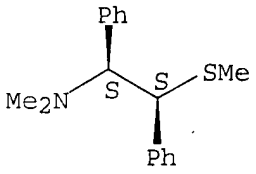
Relative stereochemistry.



RN 97241-47-9 CAPLUS
CN Benzeneethanamine, N,N-dimethyl-β-(methylthio)-α-phenyl-,

(R*,R*)- (9CI) (CA INDEX NAME)

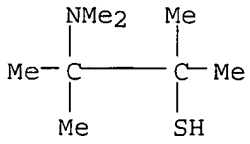
Relative stereochemistry.



L13 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1984:562548 CAPLUS
DOCUMENT NUMBER: 101:162548
TITLE: Substituted cysteamine ligands and their complexes with molybdenum(VI)
AUTHOR(S): Corbin, James L.; Miller, Kenneth F.; Pariyadath, Narayanakutty; Heinecke, Jay; Bruce, Alice E.; Wherland, Scot; Stiefel, Edward I.
CORPORATE SOURCE: Charles F. Kettering Res. Lab., Yellow Springs, OH, 45387, USA
SOURCE: Inorganic Chemistry (**1984**), 23(21), 3404-12
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB New bidentate cysteamine-based ligands containing Me-substituted C and N atoms were prepared Together with known ligands the following complete set has now been prepared: NH2CH2CH2SH, MeNHCH2CH2SH, Me2NCH2CH2SH, NH2C(CH3)2CH2SH, MeNHC(CH3)2CH2SH, Me2NC(CH3)2CH2SH, NH2CH2C(CH3)2SH, MeNHCH2C(CH3)2SH, Me2NCH2C(CH3)2SH, NH2C(CH3)2C(CH3)2SH, MeNHC(CH3)2C(CH3)2SH, and Me2NC(CH3)2C(CH3)2SH. Five of the ligands in this series are new, and their preparation is reported in detail. Also RNHCH2C(CH3)2SH ligands (R = iso-Pr and iso-Bu) are reported for the 1st time. These ligands, LH, were reacted in MeOH with MoO2(acac)2 (Hacac = acetylacetone). In most cases MoO2L2 resulted. However, in some cases this complex appears to be unstable. The prepns. and spectroscopic properties of the complexes are reported. The low values of ν(Mo-O) for some of the complexes are correlated either with H bonding or with the presence of a skew-trapezoidal-bipyramidal structure. Likewise, electronic absorption spectra differ for complexes with octahedral as opposed to skew-trapezoidal-bipyramidal structures. For a given complex, 17O and 1H NMR spectroscopies are consistent with adoption in solution of the same octahedral or skew-trapezoidal-bipyramidal structure that is found in the solid state. Further, the skew-trapezoidal-bipyramidal complexes display temperature-dependent NMR spectra that are interpreted in terms of configurational averaging probably caused by Mo-N bond cleavage.

IT **91229-44-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 91229-44-6 CAPLUS
CN 2-Butanethiol, 3-(dimethylamino)-2,3-dimethyl-, hydrochloride (9CI) (CA INDEX NAME)



● HCl

L13 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1982:216922 CAPLUS
DOCUMENT NUMBER: 96:216922
TITLE: Thioammonium ions. Azasulfenylation reactions
AUTHOR(S): Caserio, Marjorie C.; Kim, Jhong K.
CORPORATE SOURCE: Dep. Chem., Univ. California, Irvine, CA, 92717, USA
SOURCE: Journal of the American Chemical Society (**1982**), 104(11), 3231-3
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:216922

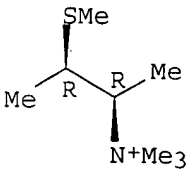
AB Attempts to prepare elusive (alkylthio)ammonium ions have given evidence for their formation as reactive intermediates in alkylation of sulfenamides and in the sulfenylation of amines. In the presence of alkenes, (alkylthio)ammonium ions are trapped as 1-ammonium-2-thio adducts formed by anti-addition These same adducts were obtained more conveniently in 2 steps: addition of (alkylthio)sulfonium ions to the alkene, followed by displacement of the sulfonium group by an amine nucleophile. The displacement step proceeds by the reversible dissociation of 1-sulfonium-2-thio adducts to episulfonium ions. The displacement reaction is general because the episulfonium ion can be trapped by a variety of nucleophiles.

IT **81206-95-3P 81206-97-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 81206-95-3 CAPLUS
CN 2-Butanaminium, N,N,N-trimethyl-3-(methylthio)-, (R*,R*)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

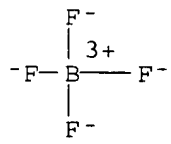
CRN 81206-94-2
CMF C8 H20 N S

Relative stereochemistry.



CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

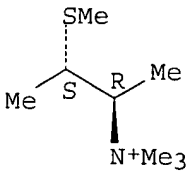


RN 81206-97-5 CAPLUS
CN 2-Butanaminium, N,N,N-trimethyl-3-(methylthio)-, (R*,S*)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

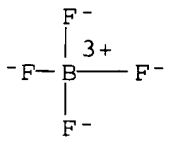
CRN 81206-96-4
CMF C8 H20 N S

Relative stereochemistry.



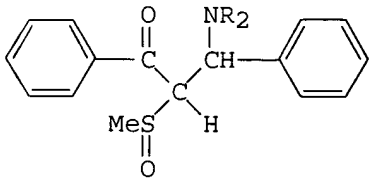
CM 2

CRN 14874-70-5
CMF B F4
CCI CCS

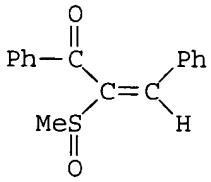


L13 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1979:574952 CAPLUS
DOCUMENT NUMBER: 91:174952
TITLE: Thermolysis of Mannich bases from β-oxo sulfoxides, benzaldehyde and secondary amines
AUTHOR(S): Boehme, Horst; Clement, Bernd
CORPORATE SOURCE: Pharm.-Chem. Inst., Philipps-Univ., Marburg, 355, Fed. Rep. Ger.
SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1979), 312(6), 531-4

CODEN: ARPMAS; ISSN: 0365-6233
DOCUMENT TYPE: Journal
LANGUAGE: German
GI



I



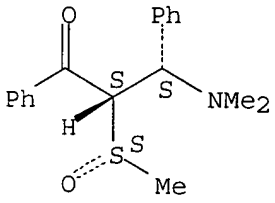
II

AB Stable Mannich bases I [R = Me, R2 = (CH2)4, CH2CH2OCH2CH2] were obtained as mixts. of 4 diastereoisomeric forms, stipulated by the 3 chiral centers, by condensation of PhCOCH2S(O)Me with PhCHO and HNR2. Amine elimination occurred on heating I (R = Me) >180° to give a single (E) diastereomer of the propenone II.

IT **71679-36-2P 71698-77-6P 71698-78-7P 71698-79-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and thermolysis of)

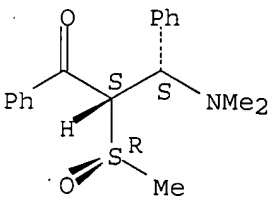
RN 71679-36-2 CAPLUS
CN 1-Propanone, 3-(dimethylamino)-2-(methylsulfinyl)-1,3-diphenyl-, [2R*(R*),3R*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 71698-77-6 CAPLUS
CN 1-Propanone, 3-(dimethylamino)-2-(methylsulfinyl)-1,3-diphenyl-, [2R*(S*),3R*]- (9CI) (CA INDEX NAME)

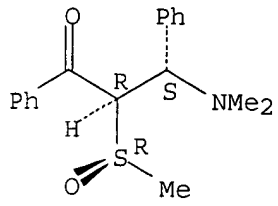
Relative stereochemistry.



RN 71698-78-7 CAPLUS
CN 1-Propanone, 3-(dimethylamino)-2-(methylsulfinyl)-1,3-diphenyl-,

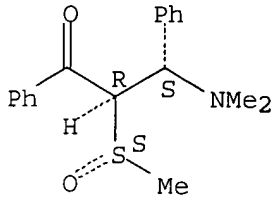
[2R*(R*),3S*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.

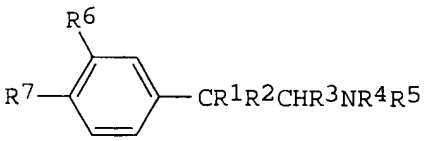


RN 71698-79-8 CAPLUS
CN 1-Propanone, 3-(dimethylamino)-2-(methylsulfinyl)-1,3-diphenyl-, [2R*(S*),3S*]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1979:97354 CAPLUS
DOCUMENT NUMBER: 90:97354
TITLE: Studies on chemical protectors against radiation. XX. Radioprotective mechanism of phenethylamine compounds
AUTHOR(S): Shinoda, Masato; Onoda, Makoto; Sato, Kazunori; Nemoto, Kyuichi; Kamogawa, Asahi
CORPORATE SOURCE: Hoshi Coll. Pharm., Tokyo, Japan
SOURCE: Yakugaku Zasshi (**1978**), 98(11), 1512-17
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI



I, R^1 and R^2 = H, OH, SH, SSO_3H, or $SC(:NH)NH_2$, R^3 and R^4 = H or Me, R^5 = H, Ac, alkyl, NH_2, or Bz, R^6 and R^7 = H or OH

AB Correlation between radioprotection by phenethylamines (I) and anoxia was

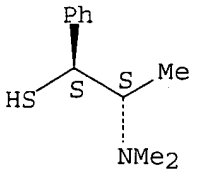
examined from their action on femoral artery blood flow and on blood pressure of the rat common carotid and isolated dorsal arteries. The radioprotection mechanism by vasoconstriction-anoxia was present in the phenethylamine-type and ephedrine-type compds., and possible participation of anoxia was suggested in some of S-ephedrine- and isothiourea-type compds. In disulfide- and thiosulfate-type compds., mechanisms other than anoxia were considered to be present.

IT **942-48-3**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(radioprotective activity of)

RN 942-48-3 CAPLUS

CN Benzenemethanethiol, α-[1-(dimethylamino)ethyl]-, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L13 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1978:31877 CAPLUS

DOCUMENT NUMBER: 88:31877

TITLE: Studies on chemical protectors against radiation. XVII. Radioprotective activities of phenethylamine compounds

AUTHOR(S): Shinoda, Masato; Ohta, Setsuko; Takagi, Yoshinari

CORPORATE SOURCE: Hoshi Coll. Pharm., Tokyo, Japan

SOURCE: Yakugaku Zasshi (**1977**), 97(10), 1117-24
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

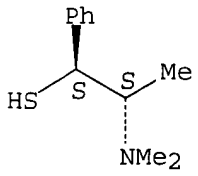
AB The relation between chemical structure and radioprotective activity was examined with 80 phenethylamine compds. and various amines. A strong radioprotective effect was shown by phenethylamine-HCl [156-28-5] and by tyramine-HCl [60-19-5], dopamine-HCl [62-31-7], norepinephrine [51-41-2], and epinephrine-HCl [55-31-2], which have a phenolic hydroxyl in their mol., but the corresponding amino acids were ineffective. Only a weak effect was shown by the ephedrine isomers, but a markedly strong effect was shown by compds. with a side chain substituted with SH, isothiourea, or thiosulfuric acid, and by the S-S ephedrine compds. Comparison of the isomers of these compds. showed that the L-erythro type compds. were more effective.

IT **942-50-7**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(radioprotective activity of)

RN 942-50-7 CAPLUS

CN Benzenemethanethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L13 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:410290 CAPLUS
DOCUMENT NUMBER: 63:10290
ORIGINAL REFERENCE NO.: 63:1821h,1822f-h,1823a-c
TITLE: Potential radiation-protective agents. III. Mercapto analogs related to ephedrine
AUTHOR(S): Bhat, K. Venkatramana; McCarthy, Walter C.
CORPORATE SOURCE: Univ. of Washington, Seattle
SOURCE: Journal of Pharmaceutical Sciences (**1965**), 54(2), 225-8
CODEN: JPMSAE; ISSN: 0022-3549
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 63:10290

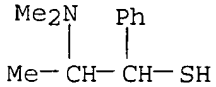
AB cf. CA 62, 5214f. Since certain sympathomimetic amines have been shown to possess radiation protective activity, the mercapto analogs related to ephedrine were selected for investigation. (+)-PhCHClCHMeNHMe.HCl (I.HCl) (19 g.) and 21.4 g. Na2S2O3.5H2O dissolved in 40 ml. hot H2O and the solution let stand 1 hr., heated 2 hrs. on a water bath, and cooled gave 20.5 g. Bunte salt PhCH(S2O3-)CHMeN+H2Me (II), m. 186-7° (H2O), [α]25D 221° (c 1, H2O). To 22 g. (+)-I.HCl in 150 ml. anhydrous MeOH was added 23 ml. MeOH-MeONa (10% Na weight/volume), followed by MeCOSNa solution [prepared from 7.5 ml. MeCOSH and 23 ml. MeOH-MeONa (10% Na weight/volume)], the mixture refluxed 3 hrs. and filtered, and the filtrate evaporated in vacuo (rotary evaporator) to give 9.5 g. (+)-PhCH(SH)CHMeNMeAc (III), m. 112-13° (dilute EtOH), [α]25D 190° (c 1, EtOH). Oxidation of (+)-III with iodine gave (+)-(AcMeNCHMeCHPhS)2 (IV), m. 172-3° (dilute EtOH), [α]25D 390° (c 1, 95% EtOH). (+)-III (5.6 g.) in 50 ml. EtOH refluxed 3 hrs. with 25 ml. concentrated HCl and the solution evaporated in vacuo (rotary evaporator) gave 4.5 g. unchanged (+)-III, m. 112-13° (dilute EtOH). (+)-III (5.6 g.) in 100 ml. 20% aqueous NaOH refluxed 24 hrs., cooled, and saturated with CO2gave [by air oxidation of (+)-III] 3.2 g. (+)-IV, m. 172-3° (dilute EtOH). (+)-IV (4.5 g.) extracted from the thimble of a Soxhlet extractor by a refluxing solution of 1.8 g. LiAlH4in 275 ml. Et2O [after 72 hrs. all (+)-IV had been extracted], 0.9 ml. H2O added dropwise with stirring, then 4.9 ml. concentrated HCl, the precipitate filtered off, extracted with Et2O, the extract filtered, the combined filtrates dried and evaporated in vacuo (rotary evaporator), and the semisolid residue recrystd. (EtOH) gave 2 g. (EtMeNCHMeCHPhS)2, m. 160-1°, [α]25D 715° (c 1, C6H6). (+)-I.HCl (22 g.) in 200 ml. absolute EtOH treated with 46 ml. EtOH-EtONa (5% Na weight/volume), followed by 16 g. EtOCS2K, and the mixture heated 3 hrs. on a steam bath and worked up gave 6

g. (-)-3,4-dimethyl-5-phenylthiazolidine-2-thione (V), m. 65-6° (iso-Pr2O), [α]25D -155° (c 1, EtOH), which was resistant to hydrolysis by boiling 48% HBr. (-)-V (8 g.) in 200 ml. anhydrous Et2O added dropwise to 3.79 g. LiAlH4 in 100 ml. Et2O and the solution refluxed 90 hrs., hydrolyzed by adding dropwise 7.2 ml. H2O and 9.7 ml. concentrated HCl, and worked up gave 4.5 g. (+)-PhCH(SH)CHMeNMe2, m. 75-6° (absolute EtOH), [α]25D 150° (c 1, 0.1N HCl), which oxidized in EtOH with 1% iodine solution gave (+)-(Me2NCHMeCHPhS)2, m. 196-7° (EtOH), [α]25D 300° (c 1, 0.1N HCl). Chloral (15 g.) added dropwise to 16.5 g. (-)-ephedrine (VI) with stirring and ice cooling and the mixture stirred 2 hrs. at room temperature and concentrated in vacuo (rotary evaporator) gave a mixture of oil and crystalline solid; recrystn. of the solid from absolute EtOH gave 1 g. (-)-VI.HCl, m. 217-18°; distillation of the oil gave 6 g. N-formyl-(-)-ephedrine (VII), b1 168-74°, ν 1665 cm.-1 Excess SOCl2added dropwise to VII with stirring and ice cooling and the mixture stirred 1.5 hrs. at room temperature and worked up gave (+)-pseudoephedrine-HCl (VIII.HCl), m. 182-3°, [α]25D 60° (c 1, H2O). SOCl2 (1.13 ml.) added dropwise to an ice cold solution of 2.07 g. N-acetylephedrine in 100 ml. CHCl3 and the mixture stirred 30 min. at room temperature, heated 30 min. on a water bath, and worked up gave 1.5 g. O-acetyl-(+)-pseudo-ephedrine-HCl, m. 185-6° (iso-PrOH), [α]25D 98° (c 1, H2O). A mixture of 10.7 g. (-)-VI.H2SO4and 12 g. 4-MeC6H4SO2Cl (IX) shaken with 60 ml. 10% aqueous NaOH and cooled in ice gave 13 g. N-p-tolylsulfonyl-(-)-ephedrine (X), m. 117-18° (60% EtOH), [α]25D -27.5° (c 1, 95% EtOH), ν 3570 cm.-1 Similar tosylation of VIII.HCl gave 84% N-p-tolylsulfonyl-(+)-pseudo-ephedrine, m. 93-4.5°, [α]25D 25° (c 1, 95% EtOH). X (3.2 g.) and 2.5 g. IX in 8 ml. C5H5N stirred 4 hrs. at room temperature and worked up gave 94% unchanged X, m. 117-18°. When the mixture was heated at 80°, unchanged X was also recovered. Refluxing the mixture gave an oil, which could not be crystallized Neither II, when administered to mice in a dosage of 51-150 mg./kg., nor 3,4-dimethyl-5-phenyl-2-iminothiazolidine-HCl (McCarthy and Ho, CA 56, 8612f), when administered to mice in a dose of 50 mg./kg, or less, showed protective activity against radiation.

IT **91341-40-1**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, (+)-
(preparation of)

RN 91341-40-1 CAPLUS

CN α-Toluenethiol, α-[1-(dimethylamino)ethyl]- (6CI, 7CI) (CA INDEX NAME)



L13 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:74011 CAPLUS
DOCUMENT NUMBER: 62:74011
ORIGINAL REFERENCE NO.: 62:13088a-d
TITLE: 1-Substituted 2-aminoethane derivatives
INVENTOR(S): Takamatsu, Hideji; Nishimura, Haruki
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd.
SOURCE: 2 pp.
DOCUMENT TYPE: Patent

LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 39022953		19641015	JP	19610415 <--

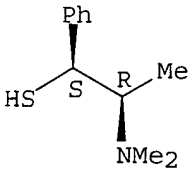
AB A mixture of 4 g. erythro-1-phenyl-1-dimethylamino-2-chloropropane-HCl (I) and 5.9 g. K thioacetate is refluxed in 60 cc. MeOH 30 min. to give 2.0 g. erythro-1-phenyl-1-mercapto-2-dimethylaminopropane (Ia), b7 109-12°. I (1.9 g.) is refluxed in 30 cc. 10% NaOH 2.5 hrs. to give 1.1 g. erythro-1-phenyl-2-dimethylaminopropanol (hydrochloride m. 206-7°). I (3.3 g.) is heated with 3.55 g. Na2S2O3, in 10 cc. H2O with steam 15 min. to give erythro-1-phenyl-2-dimethylaminopropane-1-thiosulfuric acid (II) m. 207-8° (decomposition). II (3 g.) is refluxed in 30 cc. 10% HCl 1.5 hrs., the product alkalized with Na2CO3 and extracted with ether to give 1.8 g. Ia, b3 80°. Similarly, other compds. prepared were (starting material, reagent and yield, name, and m.p. of the product given): 1-phenyl-1-dimethylamino-2-chloroethane-HCl (III) 1.5 g., K thioacetate, 1.2 g. 1-phenyl-1-mercapto-2-dimethylaminoethane-HCl, 190° (decomposition); III 8 g., Na2S2O3, 8 g., 1-phenyl-2-dimethylaminoethane-1-thiosulfuric acid, 208° (decomposition); III 2 g., Na2S reagent (7.2 g. Na2S + 10 cc. H2O + 20 cc. MeOH saturated with H2S) (reaction condition heated with steam 30 min.), 1.1 g., 1-phenyl-1-mercapto-2-dimethylaminoethane hydrochloride, 191° (decomposition); III 1 g., 10% NaOH, 0.3 g., 1-phenyl-2-dimethylaminoethanol-HCl, --; threo-1-phenyl-1-methylamino-2-chloropropane-HCl (IV) 1 g., Na2S reagent, 0.6 g., threo-1-phenyl-1-mercapto-2-methylaminopropane, -- (b2 93-6°); IV 5 g., Na2S2O3, 4 g., threo-1-phenyl-2-methylaminopropane-1-thiosulfuric acid (V), 190° (decomposition); erythro isomer of IV 1.85 g., Na2S2O3, 1.7 g. erythro isomer of V, 239° (decomposition); erythro isomer of IV 1.3 g., K thioacetate, acetyl derivative (VI) of erythro-1-phenyl-1-mercapto-2-methylaminopropane (VII), -- (VI is heated with 20% HCl in a sealed tube at 140-5° 3 hrs. to give 0.4 g. VII, b6 104°). These compds. are useful as antispasmodics.

IT **942-47-2**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, erythro-
(preparation of)

RN 942-47-2 CAPLUS

CN α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:8905 CAPLUS
DOCUMENT NUMBER: 62:8905
ORIGINAL REFERENCE NO.: 62:1588c-e
TITLE: Phenylmercaptoalkylamines. IV. Configurations of N-alkyl-1-phenyl-2-chloropropylamines and their

rearrangements with nucleophilic reagents
AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji
CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan
SOURCE: Yakugaku Zasshi (**1964**), 84(9), 817-24
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

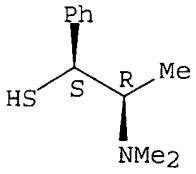
AB Treatment of DL-erythro-1-methylamino-1-phenyl-2-propanol (I) with SOCl2 gives erythro-N-methyl-1-phenyl-2-chloropropylamine-HCl (II), m. 210° (decomposition), while treatment of I with PCl5 gives the corresponding threo compound (IIa), m. 150-3°. Na2S2O3 and II and IIa gives erythro-1-phenyl-2-methylaminopropylthiosulfonic acid (III) [m. 239° (decomposition)] and the corresponding threo compound (IIIa) [m. 199-200° (decomposition)], resp. This reaction proceeds with two Walden inversions via the intermediate aziridinium compound Treatment of II and IIa with NaOH affords DL-threo-3-phenyl-1,2-dimethylaziridine (picrate m. 142-4°) and the corresponding erythro compound (picrate m. 97.5-8.5°), resp. Also is prepared erythro-N,N-dimethyl-1-phenyl-2-chloropropylamine-HCl (m. 169-70°) by chlorination of erythro-1-dimethylamino-1-phenyl-2-propanol-HCl with PCl5; no threo-type Cl derivative is obtained.

IT **942-47-2**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, erythro-
(preparation of)

RN 942-47-2 CAPLUS

CN α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



L13 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1965:8904 CAPLUS
DOCUMENT NUMBER: 62:8904
ORIGINAL REFERENCE NO.: 62:1588a-c
TITLE: Phenylmercaptoalkylamines. III. Hofmann degradation of 1-phenyl-2-dimethylaminopropanethiol quaternary salts
AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji
CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan
SOURCE: Yakugaku Zasshi (**1964**), 84(9), 811-17
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Na2S2O3 and L-(+)-threo-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, followed by hydrolysis, gave (+)-1-phenyl-2-dimethylaminopropanethiol (I), which was then converted into the methiodide and treated with NaOH to form (+)-1,2-epithiopropylbenzene (II), b10 100°, which was polymerized to give a polymer, m. 255-6°. Treatment of D-(+)-erythro-1,2-epoxypropylbenzene with KSCN gave L-(-)-erythro-1,2-epithiopropylbenzene, b7 92-3°, [α]20D-21.4° (c 2.21, MeOH), which was found to be the antipode of II. II belongs to the D-(+)-erythro series and I,

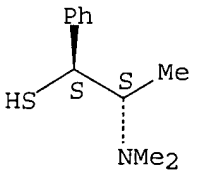
to the L-(+)-threo series. The (-)-amino thiol, similarly derived from L-(-)-erythro-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, was found to belong to the L-(-)-erythro series and that D-(+)-threo-1,2-epithiopropylbenzene (III) is derived from it. The steric configuration of II and III was also determined from their N.M.R. spectra. Hofmann degradation of the quaternary salt of 1-phenyl-2-dimethylaminoethanethiol also gave the same result. II and III underwent desulfurization by heating to give trans-β-methylstyrene.

IT **942-50-7**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, L(+)-threo-
(preparation of)

RN 942-50-7 CAPLUS

CN Benzenemethanethiol, α-[1-(dimethylamino)ethyl]-, hydrochloride, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L13 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1965:8903 CAPLUS

DOCUMENT NUMBER: 62:8903

ORIGINAL REFERENCE NO.: 62:1587h,1588a

TITLE: Phenylmercaptoalkylamines. II. Configuration of 1-phenyl-2-alkylaminopropanethiol

AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji

CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan

SOURCE: Yakugaku Zasshi (**1964**), 84(9), 806-11
CODEN: YKKZAJ; ISSN: 0031-6903

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

AB From the strength of the H bond between N and SH in the ir absorption spectra of (+)- (I) and (-)-1-phenyl-2-dimethylaminopropanethiol (Ia), obtained by treating Na2S2O3 with L-(+)-threo- (II) and L-(-)-erythro-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl (IIa) followed by hydrolysis, it was assumed that I belongs to the threo series and Ia, to the erythro series. I is also obtained by treating AcSK or NaSH with II or by treating (NH2)2CS with II followed by alkali treatment of the isothiuronium salt formed. Similarly, the steric configurations of 2 1-phenyl-2-methylaminopropanethiols and 2-imino-3,4-dimethyl-5-phenylthiazolidines, derived from L-(+)-threo-(III) and L-(-)-erythro-N-methyl-1-chloro-1-phenyl-2-propylamine hydrochlorides (IIIa) by use of foregoing reagents, were determined Use of nucleophilic reagents to II, IIa, III, and IIIa afforded derivs. without change in their steric configuration.

IT **942-48-3**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, L(+)-threo- **942-49-4**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, L(-)-erythro- **942-50-7**,

LANGUAGE: Unavailable
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3131189		19640428	US	19611016 <--

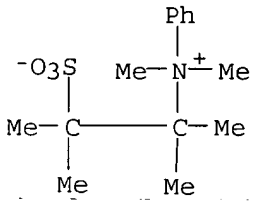
GI For diagram(s), see printed CA Issue.

AB Carbyl sulfate (I), prepared by the reaction of 2 moles SO3 and 1 mole ethylene, reacted with a tertiary amine to form betaines. Thus 1.5 g. pyridine (II) in 10 ml. ethylene dichloride was added to 3 g. I in 30 ml. ethylene dichloride (the reaction was exothermic), the liquid decanted from the precipitate, and the precipitate covered with petr. ether and cooled to give IIa (R = R1 = H), m. 250-5° (HCONMe2). I was also treated with the following to form betaines: quinoline, acridine, trimethylamine, and dimethylaniline (III). Also reported without details were: IIa (R = Ph, R1 = H); Et3NCHEtCH2SO3; IIa (R = R1 = Me); and PhNMe2CMe2CMe2SO3. These compds. are useful intermediates for the preparation of detergents. (Cf. U.S. 2,666,788, or Brit. 686,061.)

IT **97176-62-0**, Ammonium, dimethylphenyl(1,1,2-trimethyl-2-sulfopropyl), hydroxide, inner salt
(preparation of)

RN 97176-62-0 CAPLUS

CN Dimethylphenyl(1,1,2-trimethyl-2-sulfopropyl)ammonium hydroxide, inner salt (7CI) (CA INDEX NAME)



=> d l14 ibib abs hitstr tot

L14 ANSWER 1 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2001:821889 CAPLUS
DOCUMENT NUMBER: 136:118295
TITLE: Stereoselective synthesis of δ-lactones from 5-oxoalkanals via one-pot sequential acetalization, Tishchenko reaction, and lactonization by cooperative catalysis of samarium ion and mercaptan
AUTHOR(S): Hsu, Jue-Liang; Fang, Jim-Min
CORPORATE SOURCE: Department of Chemistry, National Taiwan University, Taipei, 106, Taiwan
SOURCE: Journal of Organic Chemistry (2001), 66(25), 8573-8584
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB By the synergistic catalysis of samarium ion and mercaptan, a series of 5-oxoalkanals was converted to (substituted) δ-lactones in efficient and stereoselective manners. This one-pot procedure comprises a sequence

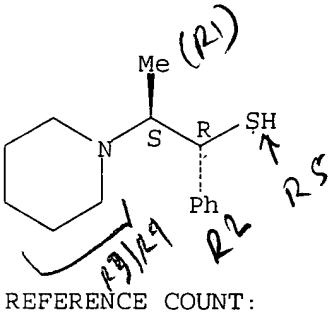
of acetalization, Tishchenko reaction and lactonization. The deliberative use of mercaptan, by comparison with alc., is advantageous to facilitate the catalytic cycle. The reaction mechanism and stereochem. are proposed and supported by some exptl. evidence. Such samarium ion/mercaptan cocatalyzed reactions show the feature of remote control, which is applicable to the asym. synthesis of optically active δ-lactones. This study also demonstrates the synthesis of two insect pheromones, (2S,5R)-2-methylhexanolide and (R)-hexadecanolide, as examples of a new protocol for asym. reduction of long-chain aliphatic ketones.

IT **166031-49-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(one-pot sequential acetalization, Tishchenko reaction, and lactonization by the promotion of samarium ion and mercaptans in stereoselective synthesis of δ-lactones from 5-oxoalkanals)

RN 166031-49-8 CAPLUS

CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 104 THERE ARE 104 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 2 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:508661 CAPLUS

DOCUMENT NUMBER: 135:256816

TITLE: A purely synthetic, diversity amenable version of norephedrine thiols for the highly enantioselective diethylzinc addition to aldehydes

AUTHOR(S): Jimeno, Ciril; Moyano, Albert; Pericas, Miquel A.; Riera, Antoni

CORPORATE SOURCE: Unitat Recerca Sintesi Asimetrica, Dep. Quim. Org., Universitat de Barcelona, Barcelona, E-08028, Spain

SOURCE: Synlett (**2001**), (7), 1155-1157
CODEN: SYNLES; ISSN: 0936-5214

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:256816

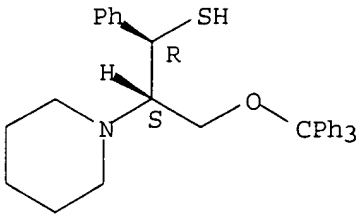
AB A new β-amino thiol arising from purely synthetic yet enantiopure amino alcs. has been prepared and successfully used in the addition of diethylzinc to aromatic aldehydes, yielding secondary alcs. in ee's up to 99%.

IT **361543-74-0P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(enantioselective diethylzinc addition to aldehydes catalyzed by β-amino thiols)

RN 361543-74-0 CAPLUS

CN 1-Piperidineethanethiol, α-phenyl-β-[(triphenylmethoxy)methyl]-, (αR,βS)- (9CI) (CA INDEX NAME)

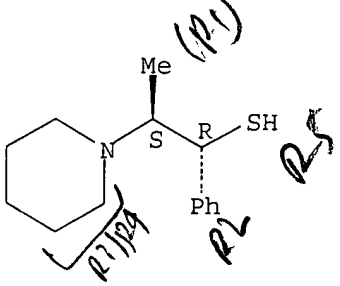
Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 3 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:296019 CAPLUS
DOCUMENT NUMBER: 130:312007
TITLE: A concise synthesis of unnatural (+)-5-epi-nojirimycin-δ-lactam via asymmetric reduction of a meso-imide
AUTHOR(S): Kang, Jahyo; Lee, Choon Woo; Lim, Geun Jho; Cho, Byung Tae
CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Tetrahedron: Asymmetry (**1999**), 10(4), 657-660
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:312007
AB Nojirimycin-δ-lactam skeleton was synthesized by asym. reduction of a cyclic triacetyloxy meso imide with a chiral β-amino thiol ligand. The resulting product was converted to unnatural (+)-5-epi-nojirimycin-δ-lactam.
IT **166031-49-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(a concise synthesis of unnatural (+)-epi-nojirimycin-δ-lactam via asym. reduction of a meso-imide)
RN 166031-49-8 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

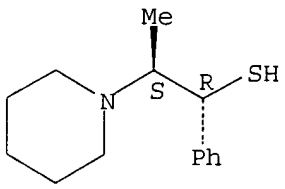
L14 ANSWER 4 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:801743 CAPLUS
DOCUMENT NUMBER: 130:153758
TITLE: Asymmetric synthesis of (diene)Fe(CO)3 complexes by a catalytic enantioselective alkylation using dialkylzincs
AUTHOR(S): Takemoto, Yoshiji; Baba, Yasutaka; Honda, Asami; Nakao, Syusuke; Noguchi, Izumi; Iwata, Chuzo; Tanaka, Tetsuaki; Ibuka, Toshiro
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences, Kyoto University, Kyoto, 606-8501, Japan
SOURCE: Tetrahedron (**1998**), 54(51), 15567-15580
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:153758

AB The reaction of meso-(2,4-hexadien-1,6-dial)Fe(CO)3 complex (1) with several alkylzincs in the presence of 50 mol% of (S)-(+)-diphenyl(1-methylpyrrolidin-2-yl)methanol proceeded with high enantiotopic group- and diastereotopic face-selectivity to give (2R,6S)-alc. complexes as major products, except in the case with dimethylzinc (>90% de and >98% ee). On the other hand, the methylation of 1 with Me2Zn proceeded with high enantioselectivity by adding 1.8 equivalent of Ti(Oi-Pr)4 in the presence of 3 mol% of (S,S)-1,2-bis(trifluoromethylsulfonamide)cyclohexane (82% de, 96% ee). The enantioselective alkylation was also applied to the kinetic resolution of racemic (sorbic aldehyde)Fe(CO)3 complex.

IT **166031-49-8**
RL: CAT (Catalyst use); USES (Uses)
(asym. synthesis of diene iron tricarbonyl complexes by catalytic enantioselective alkylation using dialkylzincs)

RN 166031-49-8 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 5 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:632164 CAPLUS
DOCUMENT NUMBER: 129:343594
TITLE: Structural chemistry of methyl- and allylpalladium(II) complexes containing chiral thioether auxiliaries
AUTHOR(S): Boog-Wick, Karin; Pregosin, Paul S.; Woerle, Michael; Albinati, Alberto
CORPORATE SOURCE: Lab. Anorganische Chem., ETH Zentrum Zuerich, Zurich,

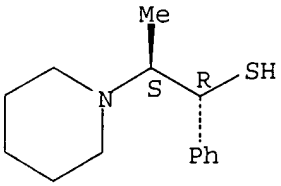
CH-8092, Switz.
SOURCE: Helvetica Chimica Acta (**1998**), 81(9), 1622-1633
CODEN: HCACAV; ISSN: 0018-019X
PUBLISHER: Verlag Helvetica Chimica Acta AG
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:343594

AB The synthesis and mol. structures of two [PdCl(Me)] complexes each containing a different chiral N,S-chelate based on {[(dihydrooxazolyl)phenyl]methyl}thioglucose backbones, i.e., chloro({2-[(4S)-4,5-dihydro-4-isopropyloxazol-2-yl-κN]phenyl}methyl 2,3,4,6-tetra-O-acetyl-1-(thio-κS)-β-D-glucopyranoside)methylpalladium(II) and a [Pd(η3-C3H5)(PS)]+ cation in which the P,S-chelate stems from a phosphinoferrocene and thioephedrine-derived thioether donor as well as [(S)-1-(diphenylphosphino-κP)-2-((1R)-1-{[(1R,2S)-1-phenyl-2-(piperidin-1-yl)propyl]thio-κS}ethyl)ferrocene](η3-prop-2-enyl)palladium trifluoromethanesulfonate are reported. In the methylpalladium compds. the thioglucose-κS moiety is pseudo-axial, whereas in the allyl complex, the thioephedrine-κS moiety is markedly pseudo-equatorial. It is suggested, based on these results, that the shape (chiral pocket) of such coordinated chiral thioethers may not be readily predictable.

IT **166031-49-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of methyl- and allylpalladium complexes with chiral thioether moieties)

RN 166031-49-8 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L14 ANSWER 6 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:482774 CAPLUS
DOCUMENT NUMBER: 129:216335
TITLE: Asymmetric synthesis of a new cylindrically chiral and air-stable ferrocenyldiphosphine and its application to rhodium-catalyzed asymmetric hydrogenation
AUTHOR(S): Kang, Jahyo; Lee, Jun Hee; Ahn, Sung Hoon; Choi, Jung Sun
CORPORATE SOURCE: Department of Chemistry and Organic Chemistry Research Center, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Tetrahedron Letters (**1998**), 39(31), 5523-5526
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 129:216335

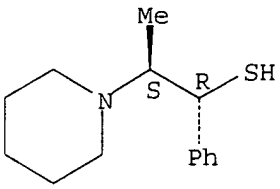
AB The novel, cylindrically chiral air-stable (S,S)-1,1'-bis(diphenylphosphino)-2,2'-di-3-pentylferrocene [(S,S)-FerroPHOS] ligand was prepared and its in situ rhodium complexes have been applied to asym. hydrogenation. High reactivity and selectivity have been realized in hydrogenation of various dehydroamino acid derivs.

IT **166031-49-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. synthesis of a new cylindrically chiral and air stable ferrocenyldiphosphine and its application to rhodium catalyzed asym. hydrogenation)

RN 166031-49-8 CAPLUS

CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 7 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:362994 CAPLUS

DOCUMENT NUMBER: 129:122430

TITLE: Examination of bidentate thiol derivatives as ligands in the Ni-catalyzed asymmetric conjugate addition of diethylzinc to enones

AUTHOR(S): Kang, Jahyo; Kim, Joo In; Lee, Jae Hoon; Kim, Hyo Jung; Byun, Yong Hun

CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (**1998**), 19(5), 601-603
CODEN: BKCSDE; ISSN: 0253-2964

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 129:122430

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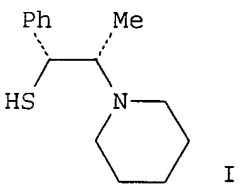


I

AB Asym. conjugate addition of diethylzinc to (E)-PhCH:CHCOPh was catalyzed by Ni(II) complexes, e.g. Ni(acac)2 or NiCl2, in presence of bidentate thiol

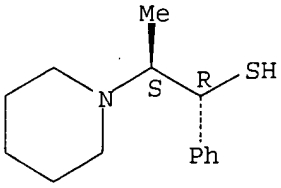
ligands, e.g. I. The major enantiomer obtained was (R)-PhCHEtCH2COPh.

IT **166031-49-8**
RL: CAT (Catalyst use); USES (Uses)
(asym. conjugate addition of diethylzinc to enones catalyzed by Ni(II) and bidentate thiol ligands)

RN 166031-49-8 CAPLUS

CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 8 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:272187 CAPLUS

DOCUMENT NUMBER: 129:54427

TITLE: The interaction of chiral amino thiols with organozinc reagents and aldehydes: a mechanism of amino thiol-catalyzed addition of organozinc reagents to aldehydes

AUTHOR(S): Kang, Jahyo; Kim, Jin Bum; Kim, Jeeyoung; Lee, Duckhwan

CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea

SOURCE: Bulletin of the Korean Chemical Society (**1998**), 19(4), 475-481
CODEN: BKCSDE; ISSN: 0253-2964

PUBLISHER: Korean Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

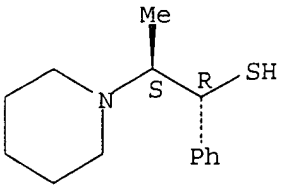
AB Details of various equilibrium involved in the reactions of oxaza- and thiazazincolidine catalysts, generated from either β-amino alc. or β-amino thiol, with benzaldehyde were studied by colligative measurements. The coordination of diethylzinc prior to the coordination of aldehyde is essential for high enantioselectivity of the thiol catalyzed reaction. The probable origin of asym. nonlinearity is also presented.

IT **166031-49-8 188711-05-9**
RL: RCT (Reactant); RACT (Reactant or reagent)
(mechanism of amino thiol-catalyzed addition of organozinc reagents to aldehydes)

RN 166031-49-8 CAPLUS

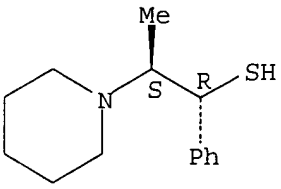
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



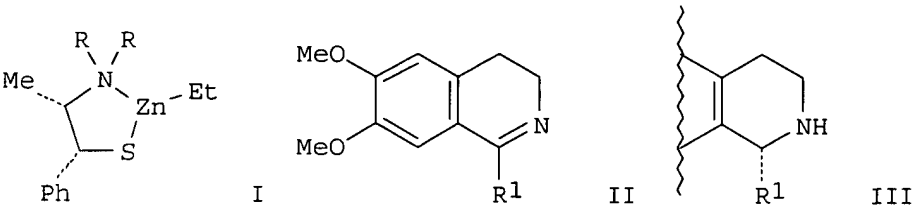
RN 188711-05-9 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 9 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:213617 CAPLUS
DOCUMENT NUMBER: 126:277632
TITLE: Enantioselective catalytic reduction of dihydroisoquinoline derivatives
AUTHOR(S): Kang, Jahyo; Kim, Jin Bum; Cho, Kwi Hyung; Cho, Byung Tae
CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Tetrahedron: Asymmetry (**1997**), 8(5), 657-660
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:277632
GI



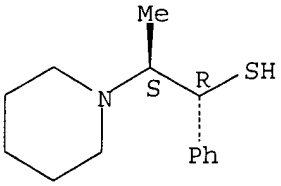
AB Zinc complexes I [RR = (CH2)5, R = Me] were shown to be excellent catalysts for enantioselective reduction of dihydroisoquinolines II (R1 = Me, 3,4-dimethoxy-, 3,4,5-trimethoxybenzyl, 3,4-dimethoxyphenyl) with

BH3·THF to the corresponding (R)-tetrahydroisoquinolines III with good enantioselectivity.

IT **166031-49-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective catalytic reduction of dihydroisoquinoline derivs.)

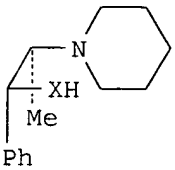
RN 166031-49-8 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 10 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:133573 CAPLUS
DOCUMENT NUMBER: 126:263720
TITLE: The effects of sulfur substitution in chiral amino thiols on the enantioselective addition of organozinc reagents to aldehydes: a novel method for estimation of free energies of dimerization in monomer-dimer equilibria
AUTHOR(S): Kang, Jahyo; Kim, Jin Bum; Kim, Jeong Whan; Lee, Duckhwan
CORPORATE SOURCE: Dep. of Chemistry, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (**1997**), (2), 189-194
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

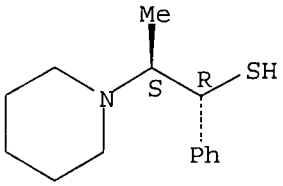
AB Differences between the thiol ligand I (X = S) and the corresponding alc. ligand (X = O) were observed in the catalytic asym. alkylation of benzaldehyde with diethylzinc. The thiol ligand was superior for reaction rate, enantioselectivity and asym. amplification. The effects of chiral amino thiols are discussed and compared with the results of chiral amino

alc. counterparts. The quant. and thermodn. aspects of the monomer-dimer equilibrium involved in thiazazincolidine or oxazazincolidine catalysts have also been studied on the basis of colligative properties.

IT **166031-49-8 188711-05-9 188711-34-4**
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(effect of sulfur substitution in chiral amino thiols on enantioselective addition of organozinc reagents to aldehydes, and colligative estimation of free energies of dimerization in monomer-dimer equilibrium)

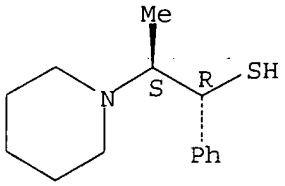
RN 166031-49-8 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



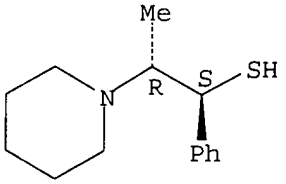
RN 188711-05-9 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 188711-34-4 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



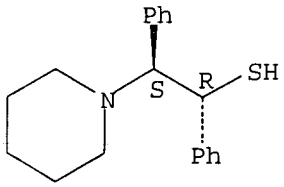
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 11 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:39785 CAPLUS
DOCUMENT NUMBER: 126:131036
TITLE: Chiral β-amino thiol catalysts for the enantioselective addition of diethylzinc to aldehydes
AUTHOR(S): Kang, Jahyo; Kim, Jeong Whan; Lee, Jun Won; Kim, Dong Soo; Kim, Joo In
CORPORATE SOURCE: Dep. Chem., Sogang Univ., Seoul, 121-742, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (**1996**), 17(12), 1135-1142
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reaction of diethylzinc with α-branched aldehydes in the presence of a catalytic amount (5 mol %) of various β-amino thiols in toluene or ether provided the corresponding secondary alcs. in outstanding ee. Detailed preparative procedure for the β-amino thiols are presented.

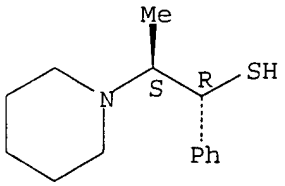
IT **160011-80-3P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(enantioselective addition of diethylzinc to aldehydes using chiral β-amino thiol catalysts)
RN 160011-80-3 CAPLUS
CN 1-Piperidineethanethiol, α,β-diphenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT **166031-49-8P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(enantioselective addition of diethylzinc to aldehydes using chiral β-amino thiol catalysts)
RN 166031-49-8 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

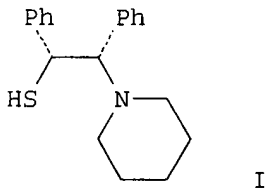
Absolute stereochemistry. Rotation (-).



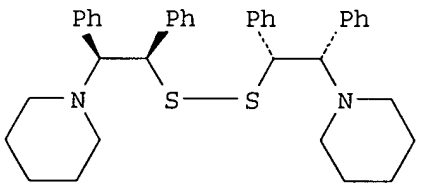
REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L14 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:194984 CAPLUS
DOCUMENT NUMBER: 122:55341
TITLE: Enantioselective addition of diethylzinc to aldehydes catalyzed by a drug-unrelated chiral amino thiol and the corresponding disulfide
AUTHOR(S): Kang, Jahyo; Kim, Dong Soo; Kim, Joo In
CORPORATE SOURCE: Department Chemistry, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Synlett (**1994**), (10), 842-4
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 122:55341
GI



I



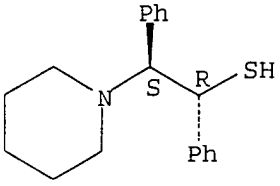
II

AB Reaction of diethylzinc with aldehydes in the presence of a catalytic amount of a β-amino thiol I (5 mol %) and the disulfide II (2.5 mol %) in toluene at 0° provided the corresponding secondary alcs. in excellent ee's.

IT **160011-80-3P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(enantioselective addition of diethylzinc with aldehydes catalyzed by chiral amino thiol and disulfide)

RN 160011-80-3 CAPLUS
CN 1-Piperidineethanethiol, α,β-diphenyl-, (αR,βS)-
(9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L14 ANSWER 13 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1995:86424 CAPLUS
DOCUMENT NUMBER: 123:142957
TITLE: Enantioselective addition of diethylzinc to

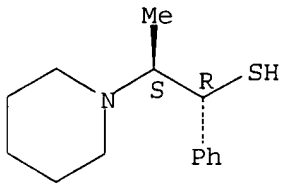
α-branched aldehydes
AUTHOR(S): Kang, Jahyo; Lee, Jun Won; Kim, Joo In
CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Journal of the Chemical Society, Chemical Communications (**1994**), (17), 2009-10
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:142957

AB Reaction of diethylzinc with α-branched aldehydes in the presence of a catalytic amount of (1R,2S)-(-)-1-phenyl-2-piperidinopropane-1-thiol provided the corresponding secondary alcs. in almost 100% enantiomeric excess.

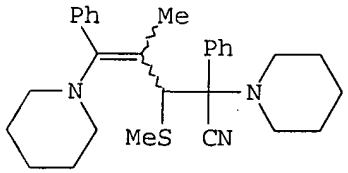
IT **166031-49-8P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(best catalyst; as ligand catalyst for enantioselective addition of diethylzinc to α-branched aldehydes)

RN 166031-49-8 CAPLUS
CN 1-Piperidineethanethiol, β-methyl-α-phenyl-, (αR,βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L14 ANSWER 14 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1993:560233 CAPLUS
DOCUMENT NUMBER: 119:160233
TITLE: Reactions of carbanions generated from 2-(dialkylamino)-2-phenylacetonitriles with disubstituted acetylenes
AUTHOR(S): Zdrojewski, Tadeusz; Jonczyk, Andrzej
CORPORATE SOURCE: Dep. Chem., Tech. Univ. (Politechnika), Warsaw, 00-662, Pol.
SOURCE: Liebigs Annalen der Chemie (**1993**), (4), 375-8
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



II

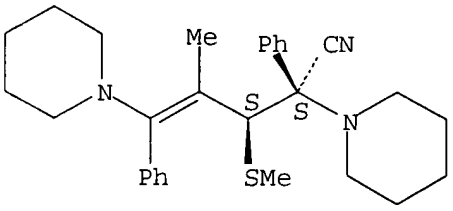
AB Reactions of aminonitriles PhCH(NR12)CN [R12 = (CH2)5, (CH2)4, (CH2)2O(CH2)2, (CH2)2S(CH2)2, (CH2)2NMe(CH2)2] with MeC.tplbond.CR2 (R2 = SMe, Ph), carried out in DMSO in the presence of powdered sodium hydroxide and benzyltriethylammonium chloride (TEBAC) as a catalyst, afford either PhC(NR12)(CN)CMe:CHR2 (I) as the E/Z isomer mixture or the pure E isomer or a mixture of I (R2 = SMe) and dipiperidinopentenenitrile II; unmasking of the carbonyl group in I [R12 = (CH2)5, R2 = Ph] and II gives ketones PhCOCMe:CHPh and PhCOCHMeCH(SMe)COPh, resp.

IT **150179-13-8P 150179-14-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cleavage of)

RN 150179-13-8 CAPLUS

CN 1-Piperidineacetonitrile, α-[2-methyl-1-(methylthio)-3-phenyl-3-(1-piperidinyl)-2-propenyl]-α-phenyl-, (R*,R*)- (9CI) (CA INDEX NAME)

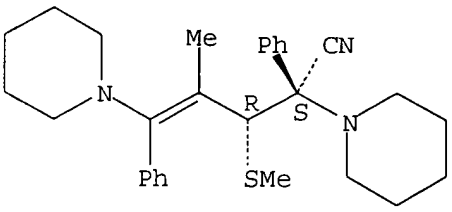
Relative stereochemistry.
Double bond geometry unknown.



RN 150179-14-9 CAPLUS

CN 1-Piperidineacetonitrile, α-[2-methyl-1-(methylthio)-3-phenyl-3-(1-piperidinyl)-2-propenyl]-α-phenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



L14 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:228476 CAPLUS
DOCUMENT NUMBER: 114:228476
TITLE: Synthesis and study of derivatives of 3-(alkylamino)-2-(methylthio)carboxylic acids
AUTHOR(S): Vidugiriene, V.; Valaviciene, J.; Rasteikiene, L.
CORPORATE SOURCE: Inst. Biokhim., Vilnius, USSR
SOURCE: Chemija (**1990**), (2), 101-6
CODEN: CHMJES; ISSN: 0235-7216
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 114:228476

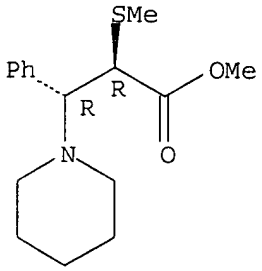
AB Treating Z-RCH:C(SMe)COX (R = Ph, Me, X = NHPh; R = Ph, X = OMe) and

RCHClCH(SMe)COX (same R, X) with 2-4 equiv HA (A = piperidino, morpholino, cyclohexylamino, ethylenimino, NHC5H11-n) gave 10 corresponding RCHACH(SMe)COX (I) as erythro-threo mixts. I had low-to-moderate toxicity and antitumor activity, with I (R = Ph, A = piperidino, X = NHPh) showing the best profile.

IT **133508-72-2P 133508-73-3P 133508-80-2P**
133508-81-3P 133612-17-6P 133612-23-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation, toxicity, and antineoplastic activity of)

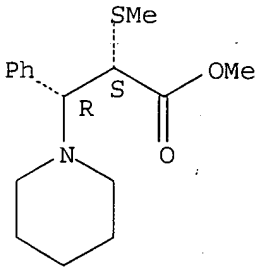
RN 133508-72-2 CAPLUS
CN 1-Piperidinepropanoic acid, α-(methylthio)-β-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



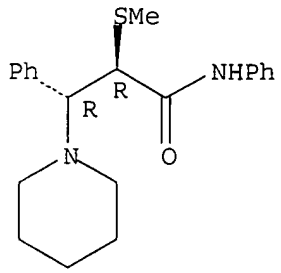
RN 133508-73-3 CAPLUS
CN 1-Piperidinepropanoic acid, α-(methylthio)-β-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



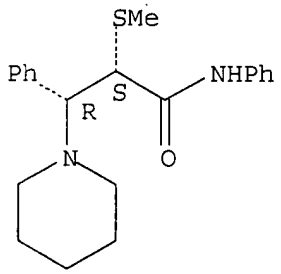
RN 133508-80-2 CAPLUS
CN 1-Piperidinepropanamide, α-(methylthio)-N,β-diphenyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



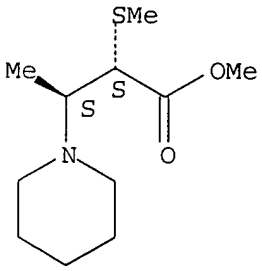
RN 133508-81-3 CAPLUS
CN 1-Piperidinepropanamide, α-(methylthio)-N,β-diphenyl-, (R*,S*)-
(9CI) (CA INDEX NAME)

Relative stereochemistry.



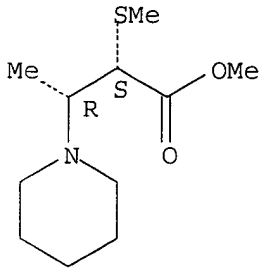
RN 133612-17-6 CAPLUS
CN 1-Piperidinepropanoic acid, β-methyl-α-(methylthio)-, methyl
ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

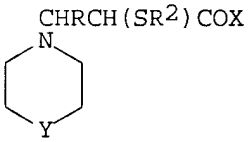


RN 133612-23-4 CAPLUS
CN 1-Piperidinepropanoic acid, β-methyl-α-(methylthio)-, methyl
ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L14 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:206268 CAPLUS
DOCUMENT NUMBER: 114:206268
TITLE: Nucleophilic addition of amines to derivatives of unsaturated acids containing 2-alkyl(phenyl)thio groups
AUTHOR(S): Talaikyte, Z.; Vidugiriene, V.; Rasteikiene, L.
CORPORATE SOURCE: Inst. Biokhim., Vilnius, USSR
SOURCE: Chemija (**1990**), (2), 93-100
CODEN: CHMJES; ISSN: 0235-7216
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI



I

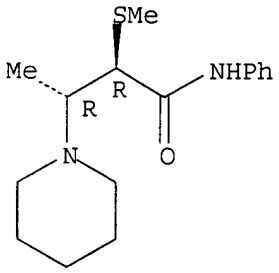
AB The title reaction of piperidine or morpholine with RCH:C(SR1)COX (R = Me, Ph; R1 = Me, Ph, CH2CH2Cl; X = NHPh, OMe) is nonstereospecific and gives mixts. of derivs. of erythro- and threo-butanoic acid I (R = Me, R2 = Me, piperidino- or morpholinoethyl; Y = CH2, O) or -phenylpropanoic acid I (R = Ph).

IT **133508-66-4P 133508-67-5P 133508-72-2P**
133508-73-3P 133508-80-2P 133508-81-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 133508-66-4 CAPLUS

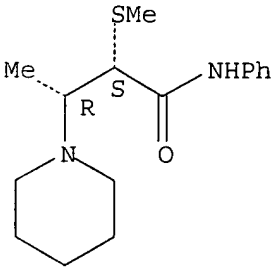
CN 1-Piperidinepropanamide, β-methyl-α-(methylthio)-N-phenyl-, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



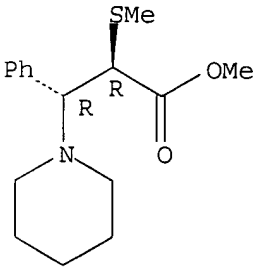
RN 133508-67-5 CAPLUS
CN 1-Piperidinepropanamide, β-methyl-α-(methylthio)-N-phenyl-, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



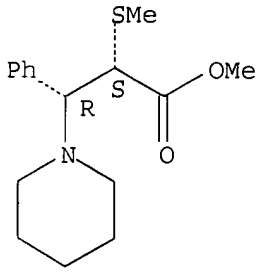
RN 133508-72-2 CAPLUS
CN 1-Piperidinepropanoic acid, α-(methylthio)-β-phenyl-, methyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



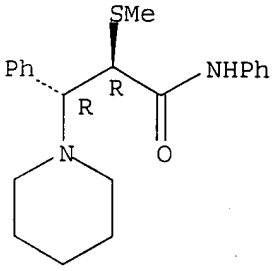
RN 133508-73-3 CAPLUS
CN 1-Piperidinepropanoic acid, α-(methylthio)-β-phenyl-, methyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



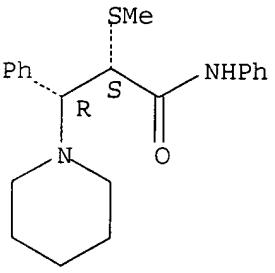
RN 133508-80-2 CAPLUS
CN 1-Piperidinepropanamide, α-(methylthio)-N,β-diphenyl-, (R*,R*)-
(9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 133508-81-3 CAPLUS
CN 1-Piperidinepropanamide, α-(methylthio)-N,β-diphenyl-, (R*,S*)-
(9CI) (CA INDEX NAME)

Relative stereochemistry.



L14 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:458617 CAPLUS
DOCUMENT NUMBER: 113:58617
TITLE: Reactions of organic anions. 168. Reactions of 2-(dialkylamino)arylacetonitriles with acetylenes under basic conditions. A simple synthesis of substituted mono- and diketones
AUTHOR(S): Zdrojewski, T.; Jonczyk, A.
CORPORATE SOURCE: Dep. Chem., Tech. Univ., Warsaw, PL-00-662, Pol.

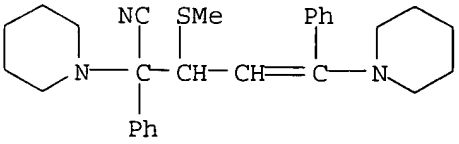
SOURCE: Synthesis (**1990**), (3), 224-33
CODEN: SYNTBF; ISSN: 0039-7881
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 113:58617

AB The reaction of RCH(CN)NR12 (I; R = Ph, 4-MeC6H4, 4-MeOC6H4; R1 = Me; NR12 = piperidino, morpholino, etc.) with R2C.tplbond.CH (II; R2 = Ph, MeS) gave R12NCR(CN)CH:CHR2 (III) and/or R12NCR(CN)CHR2CH:CRNR12; the product depended on the basicity of the amino group in III. I also added to C-1 of II (R2 = EtO) to give R12NCR(CN)C(OEt):CH2. All these products could be hydrolyzed to give mono- or diketones.

IT **128407-40-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

RN 128407-40-9 CAPLUS

CN 1-Piperidineacetonitrile, α-[1-(methylthio)-3-phenyl-3-(1-piperidinyl)-2-propenyl]-α-phenyl- (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	173.54	677.96

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-24.82	-27.01

STN INTERNATIONAL LOGOFF AT 14:27:52 ON 14 MAR 2005